

```
1 2 3 4 5 7 8 9 10

chain bonds:
    4-6 5-20 7-11 8-17 9-12 10-19 13-14 20-21

ring bonds:
    1-2 1-5 2-7 3-4 3-10 4-5 7-8 8-9 9-10

exact/norm bonds:
    4-6 5-20 7-11 8-17 9-12 10-19

exact bonds:
    1-2 1-5 2-7 3-4 3-10 4-5 7-8 8-9 9-10 13-14 20-21

isolated ring systems:
    containing 1:
```

G1:CH2,[*1]

ring nodes :

G2:CH3,Et

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 17:CLASS 19:CLASS 20:CLASS 21:CLASS

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     3 Aug 24
                 MEDLINE from 1958 to Date - Only on STN
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        Aug 28
                 DGENE GETSIM ALERT: Similarity Current-Awareness
NEWS
        Sep 7
                 Searching of Biosequences
                 Textile Technology Digest (TEXTILETECH) now available
NEWS
         Sep 11
                 on STN
                 KKF renamed DKILIT
NEWS
      7
         Sep 21
                 The Philippines Inventory of Chemicals and Chemical
NEWS
         Sep 29
                 Substances (PICCS) has been added to CHEMLIST
                 New Extraction Code PAX now available in Derwent
NEWS
        Oct 27
                 Files
                 SET ABBREVIATIONS and SET PLURALS extended in
NEWS 10
        Oct 27
                 Derwent World Patents Index files
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NEWS 11
         Oct 27
                 in Derwent Patent Files
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FULL ESTIMATED COST

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=> Uploading 09601655.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS L1 STR

$$\begin{array}{c|c} H & & & \\ \hline \\ N & & & \\ \hline \\ O & & \\ \hline \\ G2 & & \\ \end{array}$$

£H2-CH2

G1 CH2, [01]

G2 Me, Et

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 12:40:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED 49 ITERATIONS

7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: BATCH **COMPLETE**

PROJECTED ANSWERS: 561 TO 1399

7 TO 298

L2 7 SEA SSS SAM L1

=> Uploading 9601655a.str

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS
L3 STR

$$\begin{array}{c|c} H & & O \\ \hline & & \\ N & & \\ \hline & & \\$$

G1 CH2, [01] G2 Me, Et

Structure attributes must be viewed using STN Express query preparation.

=> s 13

SAMPLE SEARCH INITIATED 12:41:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 49 TO ITERATE

100.0% PROCESSED

49 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

561 TO 13

PROJECTED ANSWERS:

4 TO 200

L4

4 SEA SSS SAM L3

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 126.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 12:41:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1140 TO ITERATE

100.0% PROCESSED 1140 ITERATIONS

75 ANSWERS

SEARCH TIME: 00.00.05

L5 75 SEA SSS FUL L3

=> file ca

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY SESSION

127.20 127.35

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FILE COVERS 1967 - 27 Oct 2000 VOL 133 ISS 19 FILE LAST UPDATED: 27 Oct 2000 (20001027/ED)

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Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in CA on STN.

≈> s 15

L6 14 L5

=> s 16 and sakanaka, o?/au

21 SAKANAKA, O?/AU

L7 3 L6 AND SAKANAKA, O?/AU

=> d 17, ibib abs fhitstr, 1-3

ANSWER 1 OF 3 CA COPYRIGHT 2000 ACS L7

ACCESSION NUMBER:

131:129825 CA

TITLE:

Novel antifungal compounds and process for producing

INVENTOR(S):

Sakanaka, Osamu; Teraoka, Takeshi; Mitomo,

Koichi; Tamura, Takayoshi; Murai, Yasushi; Iinuma, Katsuharu; Kuzuhara, Kikuko; Mikoshiba, Haruki;

Taniguchi, Makoto

PATENT ASSIGNEE(S):

Meiji Seika Kaisha, Ltd., Japan

SOURCE:

PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KI	ND	DATE			APPLICATION NO.					DATE			
-,-																	
WO	9940081		Α	1	19990812			WO 1999-JP541					19990208				
	W:	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
		DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,
														MD,			
														SK,			
		TR,	TT,	UA,	UG,	US,	UZ,	VN,	YU,	ZW,	ΑM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,
		ТJ,	TM														
	RW:													CY,			
		FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,
		CM,	GΑ,	GN,	G₩,	ML,	MR,	ΝE,	SN,	TD,	TG						
AU 9924398 A1 19990823									AU 1999-24398 19990208								
PRIORITY APPLN. INFO.:									JP 1998-26257 19980206								
WO 1999-JP541 19990208												0208					
OTHER S		MARPAT 131:129825															

GΙ

AB The title compds. [I; R1 = iso-Bu, tigloyl, isovaleryl, 2-methylbutanoyl; R2 = H, arom. acyl, protecting group such substituted benzoyl, substituted

nicotinoyl; R3 = H, nitro, amino, acylamino, N,N-dialkylamino; with provisos] are prepd. Thus, UK-2A in CH2Cl2 contg. pyridine and PCl5 was refluxed for 1.5 h, the reaction mixt. was allowed to cool and then reacted with methanol for 15 h to give

(2R, 3R, 4S, 7S)-7-amino-2-benzyl-5,9-dioxa-3-isobutyryloxy-4-methyl-1,6-cyclononanedione. In an antifungal test, (2R, 3R, 4S, 7S)-7-(2-hydroxynicotinylamino)-2-benzyl-5,9-dioxa-3-isobutyryl-4-methyl-1,6-cyclononanedione (also prepd.) at 0.05 .mu.g showed potency almost double that of UK-2A against Saccharomyces cerevisiae.

IT 234112-85-7P

 ${\tt RL\colon BAC}$ (Biological activity or effector, except adverse); ${\tt IMF}$ (Industrial

Ι

manufacture); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(prepn. of UK-2A derivs. as antifungals)

RN 234112-85-7 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4,6-dimethoxy-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

REFERENCE(S):

(1) Kobe Steel Ltd; JP 07-196489 A 1969

(2) Kyowa Fermentation Industry Co, Ltd; JP 44-235 B

(3) Shimano, M; Tetrahedron 1998, V54(42), P12745 CA

(4) Suntory Ltd; JP 07-233165 A 1995

ANSWER 2 OF 3 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER:

130:193104 CA

TITLE:

Rice blast controlling agents and wheat scab

controlling agents

INVENTOR(S):

Teraoka, Takeshi; Kuzuhara, Kikuko; Mikoshiba,

Haruki;

Matsumoto, Kuniomi; Iinuma, Katsuharu; Futamura, Takafumi; Yasutake, Tetsuya; **Sakanaka, Osamu**; Mitomo, Koichi; Taniguchi, Makoto

PATENT ASSIGNEE(S):

Meiji Seika Kaisha, Ltd., Japan PCT Int. Appl., 24 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.				KIND DATE					A	PPLI	CATI	DATE					
	WO	9911127		A1		19990311			W	0 19	98-J	P387	19980831					
		W:													CN,		CZ,	DE,
															IS,			
			KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,
			NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	UA,
			UG,	US,	UZ,	VN,	YU,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM	
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,	ES,
			FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,
			CM,	GΑ,			ML,											
AU 9888878										AU 1998-88878 19980831								
										EP 1998-940634 19980831								
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	SI,	LT,	LV,	FI,	RO										
PRIO	PRIORITY APPLN. INFO.:							JP 1997-233658 1997082										
	WO 1998-JP3876 19980831																	

Ι

OTHER SOURCE(S):

MARPAT 130:193104

GΙ

These agents contain a compd. represented by formula (I) in which R1 AΒ represents alkyl or alkenyl and R2 represents hydrogen or methoxy. The compd. is highly effective in preventing rice blast and wheat scab and is not injurious to the plants. Specific compds. used in the examples are obtained by the method described in a publication presented earlier. Activities of I where R1 = iso-Pr and R2 = H (1), R1 = iso-Pr and R2 = Iso-Pr

OMe

(2), R1 = (Z)-2-butenyl and R2 = OMe(3), R1 = iso-Bu and R2 = OMe(4), and R1 = sec-Bu and R2 = OMe (5), were demonstrated.

167173-87-7 IT

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BIOL (Biological study); USES (Uses)

(as rice blast controlling agents and wheat scab controlling agents)

167173-87-7 CA RN

Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & & \\
i-Bu-C-O & Me \\
Ph-CH_2 & O & O & OH \\
O & NH-C & NH-C & OME
\end{array}$$

REFERENCE COUNT:

REFERENCE(S):

(1) Hanafi; Journal of Antibiotics 1996, V49(12), P1226 CA

(2) Suntory Ltd; JP 07-233165 A 1995

(3) Ueki; Journal of Antibiotics 1997, V50(7), P551

CA

ANSWER 3 OF 3 CA COPYRIGHT 2000 ACS 130:168617 CA

ACCESSION NUMBER: TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02 III. Absolute configuration

of

AUTHOR (S):

an antifungal antibiotic, UK-2A, and consideration of its conformation

Shibata, Kozo; Hanafi, Muhammad; Fujii, Jyunko;

Sakanaka, Osamu; Iinuma, Katsuharu; Ueki,

Masashi; Taniguchi, Makoto

CORPORATE SOURCE:

Faculty of Science, Osaka City University, Osaka,

558-8585, Japan

J. Antibiot. (1998), 51(12), 1113-1116 SOURCE:

CODEN: JANTAJ; ISSN: 0021-8820

Japan Antibiotics Research Association PUBLISHER:

Journal DOCUMENT TYPE: English LANGUAGE:

AB The abs. configuration of UK-2A (I) was detd. by the elucidation of the abs. configurations of butanolide II and the serine deriv. III, the products of alk. hydrolysis of I. The abs. configuration of UK-2A was found to be (+)-(2R,3R,4S,7S).

IT **167173-86-6**, UK 2B

RL: MSC (Miscellaneous)

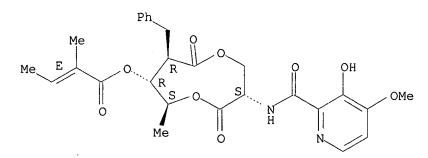
(detn. of the abs. configuration of UK-2A, an antifungal antibiotic)

RN 167173-86-6 CA

CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.



REFERENCE COUNT:

REFERENCE(S):

(1) Fuji, K; Synthesis 1975, P276 CA

(2) Hanafi, M; J Antibiotics 1996, V49, P1226 CA

- (3) Trecourt, F; Tetrahedron 1993, V49, P8373 CA
- (4) Ueki, M; J Antibitics 1996, V49, P639 CA

(5) Wasserman, H; Chem Rev 1986, V86, P845 CA ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his (FILE 'HOME' ENTERED AT 12:39:26 ON 02 NOV 2000) FILE 'REGISTRY' ENTERED AT 12:39:46 ON 02 NOV 2000 STRUCTURE UPLOADED L17 S L1 L2STRUCTURE UPLOADED L3 L44 S L3 75 S L4 FULL L5 FILE 'CA' ENTERED AT 12:42:03 ON 02 NOV 2000 14 S L5 L6 3 S L6 AND SAKANAKA, O?/AU L7=> s 16 not 17 11 L6 NOT L7 L8 => s 18 and pd < march 1998 14800117 PD < MARCH 1998 (PD<19980300) 9 L8 AND PD < MARCH 1998 L9 => d 19, ibib abs hitstr, 1-9 ANSWER 1 OF 9 CA COPYRIGHT 2000 ACS 131:214101 CA ACCESSION NUMBER: Total synthesis of the antifungal dilactone UK-2A and TITLE: analogs and their bioactivities Kamei, Noriyuki; Shibata, Tetsuo; Inoguchi, Kiyoshi; AUTHOR(S): Senda, Hisato; Ikari, Takashi; Itoh, Nobuko; Shimano, Masanao Department of Medical Chemistry and Molecular Design, CORPORATE SOURCE: Drug Discovery Research Laboratories, Kaken Pharmaceutical Co., Ltd., Japan Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (SOURCE: 1998), 40th, 679-684 CODEN: TYKYDS Nippon Kagakkai PUBLISHER: Journal DOCUMENT TYPE:

Japanese

LANGUAGE:

GI

AB UK-2A (I) which has recently been isolated from the mycelial cake of Streptomyces sp. 517-02, possesses nine-membered dilactone and a picolinic

acid moiety. The plane structure of UK-2A has been elucidated by 1H and 13C NMR analyses and chem. degrdn. studies, but the relative and abs. configurations of the four chiral centers in UK-2A still remain to be detd. UK-2A has strongly inhibited the growth of various kinds of yeasts and filamentous fungi, but its cytotoxic activities against several kinds of mammalian cells were very weak. The combination of its interesting mol. architecture and the potent antifungal activity prompted us to

the total synthesis of UK-2A. The synthesis of UK-2A has been achieved through a 12-step sequence from II in 26% overall yield. The key strategy

employed in this approach involves; (1) construction of the three consecutive chiral centers from C2 to C4 based upon the well-established Evans aldol reaction and (2) the nine-membered lactonization. The authors' synthetic route to UK-2A would permit a practical and reliable construction of UK-2A and a variety of its analogs. In order to define the selective cytotoxicities of UK-2A against yeasts and filamentous fungi, UK-2A and its analogs synthesized were subjected to the MIC evaluation and cytotoxic activity examn. compared with the ref. compds., amphotericin B and fluconazole. UK-2A has a broad antifungal spectrum, while its cytotoxicities was considerably weak compared to other substrates. The results of the UK-2A analogs suggested that the basicity of the picolinic acid moiety in UK-2A was essential for the antifungal activities and that the feature of the nine-membered dilactone contributed

to the selective cytotoxicities.

IT **167173-85-5P**, Antibiotic UK 2A

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(total synthesis of antifungal dilactone UK-2A and analogs and bioactivities)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 194931-82-3P 210426-79-2P 215798-04-2P

215798-05-3P 215798-17-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(total synthesis of antifungal dilactone UK-2A and analogs and bioactivities)

RN 194931-82-3 CA

CN Propanoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 210426-79-2 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 215798-04-2 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-05-3 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3-methoxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-17-7 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

IT 210300-07-5P 210300-13-3P 210300-18-8P 215798-00-8P 215798-10-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (total synthesis of antifungal dilactone UK-2A and analogs and bioactivities)

RN 210300-07-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 210300-13-3 CA

CN Carbamic acid,

[(3S,7R,8R,9S)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

RN 210300-18-8 CA

Propanoic acid, 2-methyl-, (3R,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-CN (phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

215798-00-8 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(1,1-CN dimethylethoxy) carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

215798-10-0 CA RN

Carbamic acid, [(3S,7R,8R,9S)-8-hydroxy-9-methyl-2,6-dioxo-7-CN (phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 2 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER: 130:3703 CA

TITLE: Total synthesis of the antifungal dilactones UK-2A

and

UK-3A: the determination of their relative and absolute configurations, analog synthesis and

antifungal activities

AUTHOR(S): Shimano, Masanao; Kamei, Noriyuki; Shibata, Tetsuo;

Inoguchi, Kiyoshi; Itoh, Nobuko; Ikari, Takashi;

Senda, Hisato

CORPORATE SOURCE: Dep. Med. Chem. Mol. Design, Drug Discovery Res.

Lab.,

SOURCE:

Kaken Pharmaceutical Co., Ltd., Minami Kawara-cho,

Yamashina-ku, Kyoto, 607-8042, Japan Tetrahedron (1998), 54(42), 12745-12774

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:3703

GΙ

The synthesis of the antifungal dilactones (I), UK-2A (R = OMe) and UK-3A (R = H), is described. In addn. to providing a workable synthetic route to these potent antifungal antibiotics, this has allowed us to det. the assignment of the relative and abs. configurations in the nine-membered ring. Furthermore, UK-2A analogs were also synthesized and evaluated for their antifungal activities and cytotoxic activities along with UK-2A, (2R, 3R, 4S, 7R)-UK-2A, UK-3A, (2R, 3R, 4S, 7R)-UK-3A, and antimycin A. The structural requirements for the selective cytotoxicity against yeasts and filamentous fungi will also be suggested.

Ι

IT 167173-85-5P, UK-2A 194931-82-3P, UK-3A 210426-79-2P 215798-04-2P 215798-05-3P 215798-17-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis, antifungal activity, cytotoxicity and abs. configuration

of

dilactones UK-2A and UK-3A)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonin-16

7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 194931-82-3 CA

CN Propanoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 210426-79-2 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 215798-04-2 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-05-3 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3-methoxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-17-7 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

210300-07-5P 210300-13-3P 210300-17-7P IT 210300-18-8P 215798-00-8P 215798-10-0P 215798-15-5P 215798-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (synthesis, antifungal activity, cytotoxicity and abs. configuration

of dilactones UK-2A and UK-3A)

210300-07-5 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-CN (phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

210300-13-3 CA RN Carbamic acid,

[(3S, 7R, 8R, 9S) - 8 - [[(1, 1-dimethylethyl)dimethylsilyl]oxy] - 9 methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 210300-17-7 CA

CN Carbamic acid,

[(3R,7R,8R,9S)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 210300-18-8 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 215798-00-8 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 215798-10-0 CA

CN Carbamic acid, [(3S,7R,8R,9S)-8-hydroxy-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CF INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-15-5 CA

CN Carbamic acid, [(3R,7R,8R,9S)-8-hydroxy-9-methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-16-6 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

36

REFERENCE(S):

(2) Barrow, C; J Antibiot 1997, V50, P729 CA (3) Brooks, B; J Comput Chem 1983, V4, P187 CA

(4) Centeno, N; Chem Phys Lett 1995, V232, P374 CA (6) Evans, D; J Am Chem Soc 1981, V103, P2127 CA (7) Evans, D; J Am Chem Soc 1982, V104, P1737 CA

ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 9 CA

ACCESSION NUMBER:

COPYRIGHT 2000 ACS 129:122477 CA

TITLE:

Enantioselective total synthesis of the antifungal dilactone, UK-2A: the determination of the relative

and absolute configurations

AUTHOR(S):

CORPORATE SOURCE:

Shimano, Masanao; Shibata, Tetsuo; Kamei, Noriyuki Dep. Medicinal Chem. Molecular Design, Drug Discovery

Res. Labs., Kaken Pharmaceutical Co., Kyoto,

607-8042,

Japan

SOURCE:

Tetrahedron Lett. (1998), 39(24), 4363-4366

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

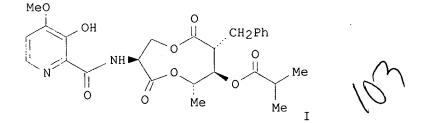
GΙ

and

Journal English

CASREACT 129:122477

Elsevier Science Ltd.



The synthesis of the antifungal dilactone, UK-2A (I), is described. In AB addn. to providing a workable synthetic route to this potent antifungal antibiotic, this has allowed us to det. the assignment of the relative

abs. configurations in the nine-membered ring.

167173-85-5P, (+)-UK-2A 210426-79-2P, 7-epi-UK-2A ΙT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (abs. configuration of UK-2A via enantioselective total synthesis)

RN 167173-85-5 CA

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 210426-79-2 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 210300-07-5P 210300-13-3P 210300-17-7P 210300-18-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (abs. configuration of UK-2A via enantioselective total synthesis)

RN 210300-07-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 210300-13-3 CA

CN Carbamic acid,

[(3S, 7R, 8R, 9S) - 8 - [[(1, 1-dimethylethyl)dimethylsilyl]oxy] - 9 -

methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 210300-17-7 CA

CN Carbamic acid,

[(3R,7R,8R,9S)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9methyl-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 210300-18-8 CA

CN Propanoic acid, 2-methyl-, (3R,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 4 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER: 128:163891 CA

TITLE: The mode of action of UK-2A and UK-3A, novel

antifungal antibiotics from Streptomyces sp. 517-02

AUTHOR(S): Ueki, Masashi; Taniguchi, Makoto

CORPORATE SOURCE: Dep. Biology, Fac. Sci., Osaka City Univ., Osaka,

558,

Japan

SOURCE: J. Antibiot. (1997), 50(12), 1052-1057

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER: Japan Antibiotics Research Association

DOCUMENT TYPE: Journal LANGUAGE: English

AB UK-2A and UK-3A are structural relatives of antimycins, which were isolated as antifungal antibiotics with little cytotoxicity that demonstrated inhibition of respiratory activity. They halve the cellular respiration of yeast within 4~5 min and the intracellular ATP content within 2~5 min. They inhibited the yeast mitochondrial respiration using .beta.-hydroxybutyrate and succinate as a respiratory substrate, but no inhibition was obsd. using ascorbate-reduced tetra-Me p-phenylenediamine as the substrate. The site of respiratory inhibition of UK-2A and UK-3A was thought to be the cytochrome bcl complex in the mitochondrial

electron

transport chain of yeast cells. They also inhibited the mitochondrial respiration of rat liver. Intact animal cells might have some system to defend themselves from the actions of UK-2A and UK-3A.

IT 167173-85-5, UK-2A 194931-82-3, Antibiotic UK-3A

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(mechanism of antifungal action of UK-2A and UK-3A)

RN 167173-85-5 CA

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 194931-82-3 CA

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CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

L9 ANSWER 5 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER:

127:217524 CA

TITLE:

UK-3A, a novel antifungal antibiotic from

Streptomyces

sp. 517-02: fermentation, isolation, structural

elucidation and biological properties

AUTHOR(S):

Ueki, Masashi; Kusumoto, Atsushi; Hanafi, Muhammad; Shibata, Kozo; Tanaka, Toshio; Taniguchi, Makoto Faculty of Science, Osaka City University, Osaka,

CORPORATE SOURCE:

558,

Japan

SOURCE:

J. Antibiot. (1997), 50(7), 551-555

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER:

Japan Antibiotics Research Association

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GΙ

AB A novel antifungal antibiotic, UK-3A (I), was obtained from the mycelial cake of Streptomyces sp. 517-02. I was very similar in structure to UK-2A, a structural relative of antimycin A. The antifungal spectrum of I

was relatively broad (MICs for yeasts and filamentous fungi: 1.56.apprx.6.25 and 0.39.apprx.1.56 .mu.g/mL, resp.). The cytotoxic

activity of I was weak (IC50: 18.apprx.100 .mu.g/mL).

194931-82-3P, Antibiotic UK 3A IT

RL: BAC (Biological activity or effector, except adverse); BOC (Biological

occurrence); BPN (Biosynthetic preparation); PRP (Properties); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(UK-3A is a novel antifungal antibiotic from Streptomyces)

194931-82-3 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

ANSWER 6 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER:

126:144017 CA

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02. II. Structural elucidation

AUTHOR(S):

Hanafi, Muhammad; Shibata, Kozo; Ueki, Masashi;

Taniguchi, Makoto

CORPORATE SOURCE:

Fac. Sci., Osaka City Univ., Osaka, 558, Japan

SOURCE:

J. Antibiot. (1996), 49(12), 1226-1231

CODEN: JANTAJ; ISSN: 0021-8820 Japan Antibiotics Research Association

PUBLISHER: Journal

DOCUMENT TYPE:

English LANGUAGE: AB

UK-2A, UK-2B, UK-2C and UK-2D, novel antibiotics produced by Streptomyces sp. 517-02, exhibit strong antifungal activity. The structures were elucidated based on spectral and chem. evidence that these compds. are the

derivs. of the nine-membered dilactone formed from serine and 4-hydroxypentanoic acid moiety.

167173-86-6P 167173-87-7P, UK 2C 167173-88-8P, ΙT UK 2D

RL: PRP (Properties); PUR (Purification or recovery); PREP (Preparation) (structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from Streptomyces sp. 517-02)

167173-86-6 CA RN

2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 167173-87-7 CA

CN Butanoic acid, 3-methyl-, $(3S, 6S, 7R, 8R)-3-[[(3-\text{hydroxy-}4-\text{methoxy-}2-\text{methoxy-}2-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-}2-\text{methoxy-}4-\text{methoxy-$

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ i-Bu-C-O \\ Ph-CH_2 \\ \hline \\ O \\ \end{array} \begin{array}{c} Me \\ O \\ NH-C \\ \hline \\ N \\ \end{array} \begin{array}{c} OH \\ OMe \\ \end{array}$$

RN 167173-88-8 CA

CN Butanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

IT 167173-85-5P

RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant);

PREP

(Preparation)

(structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from Streptomyces sp. 517-02)

167173-85-5 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

186528-19-8P, O-Methyl UK 2A IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from Streptomyces sp. 517-02)

186528-19-8 CA RN

Propanoic acid, 2-methyl-,

3-[[(3,4-dimethoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4, 9-dioxo-8-(phenylmethyl)-1, 5-dioxonan-7-yl ester, [3S-(3R*,6R*,7S*,8S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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ACCESSION NUMBER:

125:109869 CA

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02. I. Fermentation, isolation,

and biological properties

AUTHOR (S):

Ueki, Masahi; Abe, Keiichi; Hanafi, Muhammad;

Shibata,

Kozo; Tanaka, Toshio; Taniguchi, Makoto

Fac. Science, Osaka City Univ., Osaka, 558, Japan CORPORATE SOURCE:

SOURCE:

J. Antibiot. (1996), 49(7), 639-643

CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

Novel antifungal antibiotics, UK-2A (I), UK-2B (II) and a mixt. of UK-2C and UK-2D, were obtained from the mycelial cake of Streptomyces sp. AΒ 517-02. All of the UK-2 compds. were similar in structure to antimycin

The antifungal activities of of UK-2 compds. were as strong as that of Α. antimycin A. However, the UK-2 compds. demonstrated weak cytotoxicity compared to antimycin A.

167173-85-5, UK 2A 167173-86-6, UK 2B ΙT 167173-87-7, UK 2C 167173-88-8, UK 2D RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study) (UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02. I. Fermn., isolation, and biol. properties)

167173-85-5 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry.

167173-86-6 CA RN

2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-

7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 167173-87-7 CA

CN Butanoic acid, 3-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{i-Bu-C-O} & \text{Me} \\
 & \text{Ph-CH}_2 & \text{O} & \text{O} & \text{O} & \text{OH} \\
 & \text{O} & \text{NH-C} & \text{NH-C} & \text{OMe} \\
 & \text{O} & \text{O} & \text{OH} & \text{OMe} \\
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RN 167173-88-8 CA

CN Butanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

L9 ANSWER 8 OF 9 CA COPYRIGHT 2000 ACS ACCESSION NUMBER: 123:337552 CA

TITLE:

INVENTOR(S):

Fungicides manufacture with Streptoverticillium Taniguchi, Makoto; Shibata, Kozo; Abe, Keiichi;

Kodama, Tooru; Uotani, Kazumichi; Oonishi, Yoshitaka

PATENT ASSIGNEE(S):

SOURCE:

Jpn. Kokai Tokkyo Koho, 10 pp.

Suntory Ltd, Japan; Meiji Seika Co

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

KIND DATE APPLICATION NO. DATE

JP 07233165

19950905 A2

_____ JP 1994-26884

19940224 <--

OTHER SOURCE(S):

MARPAT 123:337552

GΙ

Fungicides (I: R = linear or branched aliph. (un)satd. acyl group) are AΒ manufd. by culturing Streptoverticillium sp. SAM2084. Shake-culture of Streptoverticillium sp. SAM2084 for manuf. of four I wherein R =2-methylpropanoyl (UK-2A), trans-2-methyl-2-butenoyl (UK-2B), 3-methylbutanoyl (UK-2C), and 2-methylbutanoyl (UK-2D) was shown. given were the physiol. and morphol. characteristics of the Streptoverticillium sp. SAM2084.

Ι

167173-85-5P, UK 2A 167173-86-6P, UK 2B ΙT 167173-87-7P, UK 2C 167173-88-8P, UK 2D

RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fungicides manuf. with Streptoverticillium)

167173-85-5 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

167173-86-6 CA RN

2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

167173-87-7 CA RN

Butanoic acid, 3-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ i-Bu-C-O & Me \\ Ph-CH_2 & O & O & OH \\ \hline \\ O & NH-C & NH-C \\ \hline \\ O & N$$

167173-88-8 CA RN

Butanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 9 CA COPYRIGHT 2000 ACS

ACCESSION NUMBER:

123:164736 CA

TITLE:

The structures of UK-1 and UK-2, novel antibiotics

from Streptomyces sp. 517-02

AUTHOR(S):

Hanafi, O Muhammad; Kozo, Shibata; Masaru, Kashiwada;

Masashi, Ueki; Makoto, Taniguchi

CORPORATE SOURCE:

SOURCE:

Faculty Science, Osaka City University, Japan Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (

1994), 36th, 728-35

CODEN: TYKYDS

DOCUMENT TYPE:

Journal

LANGUAGE:

Japanese

The mycelial cake was extd. with acetone, and filtered. The filtrate was concd. to give aq. soln., which was extd. with chloroform. Org. layer

was concd. to yield an oily material, followed by purifn. on silica gel column

chromatog. to give crude UK-1 and UK-2. Finally, the recrystn. of each fractions from MeOH, afforded UK-1 and UK-2. UK-1 (I), a novel metabolite, demonstrated potent cytotoxic activity against B16, Hela and P388 cells, and UK-2, novel complex of antibiotics, exhibited strong antifungal activity. Methylation of UK-1 by CH3I and anhyd. K2CO3 in dry acetone gave monomethyl ether deriv., Me-UK-1. Alk. hydrolysis of UK-1 afforded carboxylic acid deriv., DeMe-UK-1. Partial structures, A, B,

and

C were elucidated by COSY, and COLOC expts. Based on these results, the structure of UK-1 was deduced to be a novel benzoxazole dimer deriv. UK-2, novel metabolite contg. complex of antibiotics with strong antifungal activity, was purified by reverse phase HPLC, to give UK-2A,

В,

C and D. From NMR and mass spectral data, the structures of UK-2A, B, C and D were established as isobutyrate, tiglate, isovalerate, and 2-methylbutyrate of nine membered dilactone skeleton, resp. Based on the result of synthesis of hydrolysis products, the abs. configuration of

UK-2

was identified.

167173-85-5, Antibiotic UK 2A 167173-86-6, Antibiotic UK IT2B 167173-87-7, Antibiotic UK 2C 167173-88-8,

Antibiotic UK 2D

RL: PRP (Properties)

(structures of UK-1 and UK-2, novel antibiotics from Streptomyces sp. 517-02)

167173-85-5 CA RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

167173-86-6 CA RN

2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

167173-87-7 CA RN

Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 167173-88-8 CA

CN Butanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-

pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	49.24	176.59
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.36	-6.36

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```
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     FILE 'REGISTRY' ENTERED AT 12:39:46 ON 02 NOV 2000
               STRUCTURE UPLOADED
L1
              7 S L1
L2
                STRUCTURE UPLOADED
L3
              4 S L3
L4
             75 S L4 FULL
L5
     FILE 'CA' ENTERED AT 12:42:03 ON 02 NOV 2000
             14 S L5
L6
             3 S L6 AND SAKANAKA, O?/AU
L7
             11 S L6 NOT L7
T8
              9 S L8 AND PD < MARCH 1998
L9
     FILE 'CAOLD' ENTERED AT 12:44:17 ON 02 NOV 2000
=> s 15
             0 L5
L10
=> d his
     (FILE 'HOME' ENTERED AT 12:39:26 ON 02 NOV 2000)
     FILE 'REGISTRY' ENTERED AT 12:39:46 ON 02 NOV 2000
                STRUCTURE UPLOADED
L1
              7 S L1
L2
                STRUCTURE UPLOADED
L3
              4 S L3
L4
             75 S L4 FULL
L5
     FILE 'CA' ENTERED AT 12:42:03 ON 02 NOV 2000
             14 S L5
L6
               3 S L6 AND SAKANAKA, O?/AU
L7
             11 S L6 NOT L7
L8
              9 S L8 AND PD < MARCH 1998
L9
     FILE 'CAOLD' ENTERED AT 12:44:17 ON 02 NOV 2000
               0 S L5
L10
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-6.36

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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                 CAS patent coverage expanded
        Aug 21
NEWS
                 TABULATE Now Available in More STN Databases
NEWS
         Aug 24
                 MEDLINE from 1958 to Date - Only on STN
NEWS
         Aug 28
                 DGENE GETSIM ALERT: Similarity Current-Awareness
NEWS
         Sep 7
                 Searching of Biosequences
                 Textile Technology Digest (TEXTILETECH) now available
NEWS
         Sep 11
                 on STN
                 KKF renamed DKILIT
NEWS
     7
         Sep 21
                 The Philippines Inventory of Chemicals and Chemical
     8
         Sep 29
NEWS
                 Substances (PICCS) has been added to CHEMLIST
                 New Extraction Code PAX now available in Derwent
         Oct 27
NEWS
                 SET ABBREVIATIONS and SET PLURALS extended in
NEWS 10
         Oct 27
                 Derwent World Patents Index files
         Oct 27
                 Patent Assignee Code Dictionary now available
NEWS 11
                 in Derwent Patent Files
                 Plasdoc Key Serials Dictionary and Echoing added to
NEWS 12 Oct 27
                 Derwent Subscriber Files WPIDS and WPIX
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              (WINDOWS) NOW AVAILABLE
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              Direct Dial and Telecommunication Network Access to STN
NEWS PHONE
NEWS WWW
              CAS World Wide Web Site (general information)
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OTHER CA INDEX NAMES:

CN

OTHER NAMES:

2-Butenoyl chloride, 2-methyl-, (E)-

(E)-2-Methyl-2-butenoyl chloride

Tigloyl chloride (6CI, 7CI)

```
Tiglic acid chloride
CN
     STEREOSEARCH
FS
     C5 H7 C1 O
MF
        N Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, SPECINFO, TOXLIT, USPATFULL
     STN Files:
LC
          (*File contains numerically searchable property data)
      Other Sources: EINECS**
          (**Enter CHEMLIST File for up-to-date regulatory information)
Double bond geometry as shown.
                 74 REFERENCES IN FILE CA (1967 TO DATE)
                 74 REFERENCES IN FILE CAPLUS (1967 TO DATE)
                  2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
=> e isopropyl/cn
                       ISOPROPROPYL (PHENYLIMINO) ACETATE/CN
                       ISOPROPYDRIN/CN
E2
                1 --> ISOPROPYL/CN
E3
                       ISOPROPYL ((2-BROMOETHYL)THIO)ACETATE/CN
                1
                       ISOPROPYL
                1
((4-CHLOROPHENYL)AMINO)IMINOMETHYLCARBAMIMIDATE/CN
               1 ISOPROPYL ((4-METHOXYPHENYL)IMINO)ACETATE/CN
                       ISOPROPYL ((CHLOROMETHYL)THIO)ACETATE/CN
E7
               1
              1 ISOPROPYL (+)-2-CHLOROPROPIONATE/CN
1 ISOPROPYL (.+-.)-.ALPHA.-ISOCYANOPROPIONATE/CN
1 ISOPROPYL (.+-.)-3-OXOCYCLOHEXANECARBOXYLATE/CN
1 ISOPROPYL (.+-.)-CIS-CRYSANTHEMATE/CN
                       ISOPROPYL ((PERHYDROAZEPINO)METHYL)(METHYL)PHOSPHINATE/CN
E10
E11
E12
=> s e3
               1 ISOPROPYL/CN
L_2
=> d 12
      ANSWER 1 OF 1 REGISTRY COPYRIGHT 2000 ACS
L2
      2025-55-0 REGISTRY
 RN
      Ethyl, 1-methyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
      Isopropyl (6CI, 8CI)
 OTHER NAMES:
      1-Methylethyl
 CN
       2-Propyl
 CN
```

2-Propyl radical

CN

Page 3

```
CN
     iso-Propyl
CN
     iso-Propyl radical
     Isopropyl radical
CN
MF
     C3 H7
                  AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD,
LC
     STN Files:
CAPLUS,
       CASREACT, CEN, CIN, GMELIN*, PIRA, PROMT, TOXLIT, TRCTHERMO*, USPATFULL
         (*File contains numerically searchable property data)
H3C-CH-CH3
             427 REFERENCES IN FILE CA (1967 TO DATE)
               6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             427 REFERENCES IN FILE CAPLUS (1967 TO DATE)
              40 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
=> e isovaleryl.cn
                    ISOVALERY/BI
             1
E1
           988
                   ISOVALERYL/BI
E2
             0 --> ISOVALERYL.CN/BI
E3
                   ISOVALERYLACET/BI
             6
E4
                   ISOVALERYLACETATE/BI
             1
E5
                   ISOVALERYLACETIC/BI
             1
E6
                    ISOVALERYLACETO/BI
E7
             1
                    ISOVALERYLACETONE/BI
E8
                   ISOVALERYLACETOPHEN/BI
             1
E9
                   ISOVALERYLACETOPHENONE/BI
E10
             1
                   ISOVALERYLADENOSINE/BI
E11
             1
                   ISOVALERYLADRENAL/BI
             1
E12
=> s e2
           988 ISOVALERYL/BI
L3
=> d 13, 1
     ANSWER 1 OF 988 REGISTRY COPYRIGHT 2000 ACS
      254879-11-3 REGISTRY
RN
      4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-6-methoxy-7-
CN
      [[6-O-(3-methyl-1-oxobutyl)-.beta.-D-glucopyranosyl]oxy]- (9CI) (CA
INDEX
     NAME)
OTHER NAMES:
     Patuletin 7-0-(6''-isovaleryl)glucoside
FS
      STEREOSEARCH
     C27 H30 O14
MF
SR
     CA
                   CA, CAPLUS
      STN Files:
LC
Absolute stereochemistry. Rotation (+).
```

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 13:00:52 ON 02 NOV 2000)

FILE 'REGISTRY' ENTERED AT 13:00:59 ON 02 NOV 2000

E TIGLOYL/CN

L1 1 S E4

E ISOPROPYL/CN

L2 1 S E3

E ISOVALERYL.CN

L3 988 S E2

=> e isovaleryl/cn

E1	1	ISOVALEROYL-COENZYME A DEHYDROGENASE/CN
E2	1	ISOVALEROYLPENTAMETHYLBENZENE/CN
E3	1>	ISOVALERYL/CN
E4	1	ISOVALERYL ANHYDRIDE/CN
E5	1	ISOVALERYL AZIDE/CN
E6	1	ISOVALERYL CHLORIDE/CN
E7	1	ISOVALERYL COA DEHYDROGENASE/CN
E8	1	ISOVALERYL COENZYME A/CN
E9	1	ISOVALERYL DIETHYLAMIDE/CN
E10	1	ISOVALERYL FLUORIDE/CN
E11	1	ISOVALERYL ISOTHIOCYANATE/CN
E12	1	ISOVALERYL L-CARNITINE/CN

=> s e6

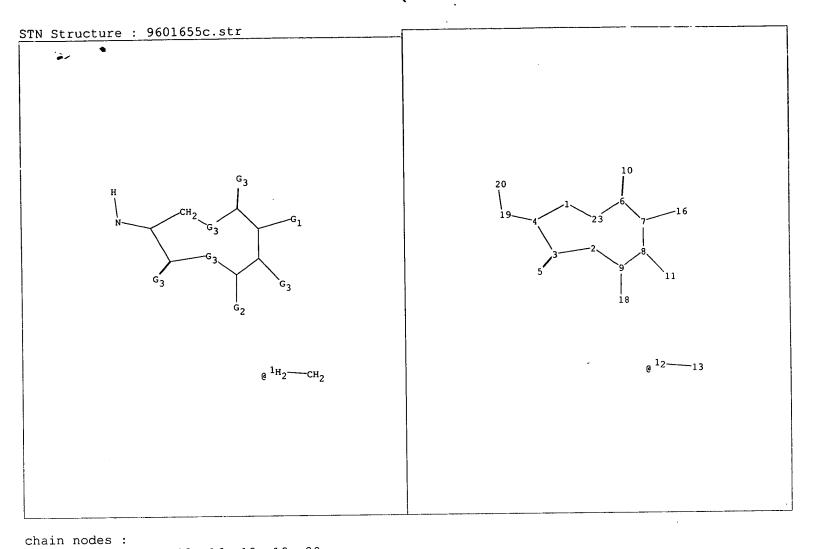
L4 1 "ISOVALERYL CHLORIDE"/CN

=> d 14

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2000 ACS RN 108-12-3 REGISTRY

```
Butanoyl chloride, 3-methyl- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
    Isovaleryl chloride (6CI, 7CI, 8CI)
CN
OTHER NAMES:
     3-Methylbutanoyl chloride
CN
     3-Methylbutyryl chloride
CN
     Isopentanoyl chloride
CN
     Isovaleric acid chloride
CN
     Isovaleric chloride
CN
     Isovaleroyl chloride
CN
     3D CONCORD
FS
MF
     C5 H9 C1 O
                  BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
     STN Files:
LC
       CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, HODOC*, IFICDB, IFIPAT,
IFIUDB,
       MRCK*, MSDS-OHS, SPECINFO, TOXLINE, TOXLIT, USPATFULL
         (*File contains numerically searchable property data)
                     DSL**, EINECS**, TSCA**
     Other Sources:
         (**Enter CHEMLIST File for up-to-date regulatory information)
Cl-C-Bu-i
             612 REFERENCES IN FILE CA (1967 TO DATE)
               1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             614 REFERENCES IN FILE CAPLUS (1967 TO DATE)
```

3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)



```
5 10 11 12 13 16 18 19 20
ring nodes:
    1 2 3 4 6 7 8 9 23
chain bonds:
    3-5 4-19 6-10 7-16 8-11 9-18 12-13 19-20
ring bonds:
    1-4 1-23 2-3 2-9 3-4 6-7 6-23 7-8 8-9
exact/norm bonds:
    1-4 1-23 2-3 2-9 3-4 3-5 4-19 6-10 6-7 6-23 7-8 7-16 8-9 8-11 9-18 12-13 19-20
isolated ring systems:
    containing 1:
```

G1:CH2,[*1]
G2:CH3,Et

G3:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS 23:Atom

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NEWS
                 MEDLINE from 1958 to Date - Only on STN
NEWS
        Aug 28
                 DGENE GETSIM ALERT: Similarity Current-Awareness
     5
        Sep 7
NEWS
                 Searching of Biosequences
                 Textile Technology Digest (TEXTILETECH) now available
NEWS
     6
        Sep 11
                 on STN
                 KKF renamed DKILIT
NEWS
     7
         Sep 21
                 The Philippines Inventory of Chemicals and Chemical
         Sep 29
NEWS
      8
                 Substances (PICCS) has been added to CHEMLIST
                 New Extraction Code PAX now available in Derwent
NEWS
      9
         Oct 27
                 Files
                 SET ABBREVIATIONS and SET PLURALS extended in
         Oct 27
NEWS 10
                 Derwent World Patents Index files
                 Patent Assignee Code Dictionary now available
         Oct 27
NEWS 11
                 in Derwent Patent Files
                 Plasdoc Key Serials Dictionary and Echoing added to
        Oct 27
NEWS 12
                 Derwent Subscriber Files WPIDS and WPIX
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              (WINDOWS) NOW AVAILABLE
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NEWS PHONE
              CAS World Wide Web Site (general information)
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١

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=> Uploading 9601655c.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS L1 STR

$$\begin{array}{c|c} & G3 \\ & & &$$

СН2—сн2

G1 CH2, [@1]

G2 Me, Et

G3 0, S

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 13:29:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5283 TO ITERATE

18.9% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

ţ

PROJECTED ITERATIONS: 101308 TO 110012 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 12 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 126.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 13:30:12 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 104836 TO ITERATE

100.0% PROCESSED 104836 ITERATIONS SEARCH TIME: 00.00.04

75 ANSWERS

0 ANSWERS

L3 75 SEA SSS FUL L1

=> file ca

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SINCE FILE TOTAL
ENTRY SESSION
126.60 126.75

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=> s 13

L4 14 L3

=> save title

ENTER L#, L# RANGE, ALL, OR (END):14

ENTER NAME OR (END):anti655/a

ENTER TITLE (NONE):broad search 11/2/00

ANSWER SET L4 HAS BEEN SAVED AS 'ANTI655/A'